

# Quantum walks with a one-dimensional coin

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Quantum walks (QWs) describe particles evolving coherently on a graph. The internal degree of freedom corresponds to a Hilbert space, called *coin system*. We consider QWs on Cayley graphs of some group  $G$ . In the literature, investigations concerning infinite  $G$  have been focused on graphs corresponding to  $G = \mathbb{Z}^d$  with coin system of dimension 2, whereas for one-dimensional coin (so called *scalar QWs*) only the case of finite  $G$  has been studied. Here we prove that the evolution of a scalar QW with  $G$  infinite Abelian is trivial, providing a thorough classification of this kind of walks. Then we consider the infinite dihedral group  $D_\infty$ , that is the unique non-Abelian group  $G$  containing a subgroup  $H \cong \mathbb{Z}$  with two cosets. We characterize the class of QWs on the Cayley graphs of  $D_\infty$  and, via a coarse-graining technique, we show that it coincides with the class of spinorial walks on  $\mathbb{Z}$  which satisfies parity symmetry. This class of QWs includes the *Weyl* and the *Dirac* QWs. Remarkably, there exist also spinorial walks that are not coarse-graining of a scalar QW, such as the *Hadamard walk*.

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## I. INTRODUCTION

Quantum walks (QWs) are the quantum version of the *classical random walks*, which made their first appearance in physics with Einstein’s seminal work on Brownian motion [1]. A peculiarity of QWs on graphs with respect to their classical counterpart is that the vertexes of the graph carry an internal degree of freedom (spin, helicity, etc.) corresponding to a finite-dimension Hilbert space, called *coin system*.

Models of QWs have been broadly studied in diverse formulations [2–7], since they revealed to be suitable both as a simulation tool—e.g. in *lattice gauge theories* [8–10]—and as a computational one—e.g. in designing *quantum algorithms* [11–13]. Recently, QWs have also been exploited as discrete models of spacetime [14–19]. Discrete-time QWs on lattices have been studied in the continuum limit in Refs. [15, 20–22], recovering Weyl, Dirac and Maxwell dynamics.

In this manuscript we consider discrete-time QWs on an infinite graph requiring *locality* and *homogeneity* of the evolution. The former implies that each site (each vertex of the graph) has a finite number of first neighbours, while the latter means the indistinguishability of the sites based on the evolution in a sense formalized in Ref. [15], where it is proved that these hypotheses amount to require the graph to be a *Cayley graph* of a finitely generated group  $G$ . Cayley graphs, as diagrammatic counterparts of groups, are convenient means to study QWs exploiting the group-theoretical machinery.

In the case of Abelian  $G$ , one can represent the walk in the wave-vectors space via the Fourier transform, resorting to the (one-dimensional) irreducible representations of  $G$ . This allows one to diagonalize the walk evolution operator and to simply solve the walk dynamics in terms of its *dispersion relations*.

The procedure is not so straightforward in the non-

Abelian case. Indeed, a method working in the general case is still lacking, due to the fact that representations of the infinite discrete non-Abelian groups are generally unknown. In Ref. [23], a novel technique allowing to tackle this issue in the case of *virtually Abelian groups* has been presented.

A virtually Abelian group  $G$  is generally a non-Abelian group with an Abelian subgroup  $H$  of finite *index* (the number of cosets of  $H$  in  $G$ ). This property enables one to define a notion of wave-vector as an invariant of the dynamics also in the non-Abelian case, thus solving the dynamics of these particular non-Abelian QWs. This technique can be viewed as a *coarse-graining* of the walk: the original virtually Abelian QW on  $G$  is unitarily equivalent to a walk on  $H$  with a larger coin system.

We will apply this method to the most elementary case of *scalar QWs*, i.e. walks with a one-dimensional coin system. This kind of walks are the most elementary ones from the point of view of the coin system, but unfortunately this does not mean that they are the easiest to treat, since their existence imposes additional constraints on the graph (see Sec. II). Scalar QWs on Cayley graph have been explored in Ref. [27], where the authors restricted the investigation to finite groups, classifying scalar QWs on Cayley graphs with two and three generators. The present investigation focuses on infinite groups. The framework of scalar QWs differs from that of staggered QWs, i.e. QWs without coin tossing, recently considered in the literature [24–26] where the walk is defined by an evolution operator that is the product of two reflections acting on the site basis.

After reviewing QWs on Cayley graphs, in Sec. III we first investigate and classify infinite Abelian scalar QWs, extending the results of Ref. [28] to any infinite Abelian group, and with arbitrary presentations. Then, in Sec. IV A, we consider the simplest case of non-Abelian group  $G$  with a subgroup  $H \cong \mathbb{Z}$  of index 2. Such a group is

the infinite dihedral group  $D_\infty$ , and we derive all its Cayley graphs admitting a scalar QW with a coarse-grained scheme having coordination number 2. All the scalar QWs on these Cayley graphs are derived in Sec. IV B. We show that their coarse-graining coincides (up to a local change of basis) with the class of QWs on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$  that are invariant under parity transformation. The walks in this class are studied via the usual Fourier-transform method and it results that they can exhibit both linear and massive dispersion relations.

## II. QWS ON CAYLEY GRAPHS

In this section we review the notion of quantum walks on Cayley graphs, previously discussed in Refs. [27, 29, 30].

Let  $G$  be a group: we can always select a *generating set*  $S_+$  for  $G$ , namely a subset  $S_+ \subseteq G$  such that any element of the group can be built as composition of elements  $g \in S_+$  and their inverses. In the following we do not assume the generating set to be *symmetric* (a generating set  $S_+$  is called symmetric if  $S_+ = S_-$ , where  $S_-$  is the set of inverses of the elements in  $S_+$ ). In order to specify a group, as well as a generating set  $S_+$ , a set  $R$  of *relators* is also needed, namely some *words* formally built by composition of elements  $g \in S_+$  and corresponding to the identity element  $e \in G$ . For example, if  $R$  is trivial, one gets the free group on  $S_+$ .

These two ingredients provide a so-called *presentation*  $G = \langle S_+ | R \rangle$  of a group. Presentations are not in one-to-one correspondence with groups: given a group  $G$ , it has in general different presentations. However, any presentation completely specifies a unique group.

Presentations of groups have a convenient geometrical representation: *Cayley graphs*. Given a group  $G$  and a generating set  $S_+$  for  $G$ , the Cayley graph  $\Gamma(G, S_+)$  is defined as the edge-colored directed graph having vertex set  $G$ , edge set  $\{(x, xg); x \in G, g \in S_+\}$ , and a color assigned to each generator  $g \in S_+$ . Besides, an edge corresponding to a generator  $g \in S_+$  is usually represented as undirected when  $g^2 = e$ . Cayley graphs are indeed in one-to-one correspondence with presentations. Relators are just closed paths over the graph, i.e. *cycles*, and conversely any cycle on the graph can be built as composition of some relators.

In the following we will consider Cayley graphs of finitely generated groups ( $|S_+| < \infty$ ) as the graphs of our quantum walks. A discrete-time quantum walk on a Cayley graph  $\Gamma(G, S_+)$  with an  $s$ -dimensional coin system ( $s \geq 1$ ) is a unitary evolution of a system with Hilbert space  $\ell^2(G) \otimes \mathbb{C}^s$  such that

$$|\psi_{g,t+1}\rangle = \sum_{h \in S_+} A_h |\psi_{gh,t}\rangle, \quad (1)$$

where  $0 \neq A_h \in M_s(\mathbb{C})$  are the *transition matrices* of the walk. In the following, we will consider  $S_+$  generally

non symmetric. In the previous literature [15] the sum in Eq. (1) was extended to  $S_+ \cup S_-$ . For this reason, for the sake of uniformity, we will explicitly name the walk *monoidal* whenever  $S_+$  is not symmetric. [31]

Considering the right regular representation  $T_g$  of the group  $G$ , whose action on  $\ell^2(G)$  is defined as  $T_g|x\rangle := |xg^{-1}\rangle$ , we can represent the QW through

$$A := \sum_{h \in S_+} T_h \otimes A_h.$$

The unitarity conditions for the walk operator  $A$  are  $AA^\dagger = A^\dagger A = T_e \otimes I_s$ ; these conditions, for a scalar QW of the form

$$A := \sum_{h \in S_+} T_h z_h$$

(where the  $z_h \in \mathbb{C}$  are called *transition scalars*), lead to the set of equations:

$$\sum_{\substack{hh'^{-1}=g \\ h \neq h'}} z_h z_{h'}^* = 0, \quad \sum_{\substack{h^{-1}h'=g \\ h \neq h'}} z_h^* z_{h'} = 0, \quad \sum_h |z_h|^2 = 1. \quad (2)$$

It is immediate to check that trivial solutions of Eq. (2) with  $A = T_h$  can occur only for monoidal walks QW with singleton  $S_+ = \{h\}$ . A necessary condition for the existence of solutions of Eq. (2) is given by the following Lemma.

**Lemma 1.** *Given a Cayley graph  $\Gamma(G, S_+)$ , a necessary condition for the existence of a scalar quantum walk  $A = \sum_{h \in S_+} T_h z_h$  on  $\Gamma(G, S_+)$  is that, for each ordered pair  $(h_1, h_2) \in S_+ \times S_+$  such that  $h_1 \neq h_2$ , there exists at least a different pair  $(h_3, h_4)$  such that  $h_1 h_2^{-1} = h_3 h_4^{-1}$ . This is called quadrangularity condition. [27]*

### A. Free Abelian QWs

The case of QWs on Cayley graphs of a free Abelian group—i.e.  $G \cong \mathbb{Z}^d$ —is the simplest to treat in order to analytically solve the dynamics, since the walk can be easily diagonalized by a Fourier transform. We will label the elements  $\mathbf{x} \in \mathbb{Z}^d$ , using the additive notation for the group composition. The right regular representation is decomposed into one-dimensional irreducible representations, since the group is Abelian. One can thus diagonalize  $T_{\mathbf{x}}$  in the wave-vector space as follows

$$|\mathbf{k}\rangle := \frac{1}{(2\pi)^{\frac{d}{2}}} \sum_{\mathbf{x}' \in \mathbb{Z}^d} e^{-i\mathbf{k} \cdot \mathbf{x}'} |\mathbf{x}'\rangle, \quad T_{\mathbf{x}} |\mathbf{k}\rangle = e^{-i\mathbf{k} \cdot \mathbf{x}} |\mathbf{k}\rangle,$$

where  $\mathbf{k}$  belongs to the *first Brillouin zone*  $\mathcal{B} \subseteq \mathbb{R}^d$ , which is the largest set that contains vectors  $\mathbf{k}$  corresponding to inequivalent elements  $|\mathbf{k}\rangle$ . The evolution operator of the walk then reads

$$A = \int_{\mathcal{B}} d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| \otimes A_{\mathbf{k}}, \quad A_{\mathbf{k}} := \sum_{h \in S_+} e^{-i\mathbf{k} \cdot \mathbf{h}} A_h,$$

where  $A_{\mathbf{k}}$  is unitary  $\forall \mathbf{k} \in \mathcal{B}$ . Being  $A_{\mathbf{k}}$  unitary, the eigenvalues are phase factors of the form  $e^{i\omega_r(\mathbf{k})}$ : the collection  $\{\omega_r(\mathbf{k})\}_{r=1,\dots,s}$  for  $\mathbf{k} \in \mathcal{B}$  are called the *dispersion relations* of the QW, and give the kinematics of the walk. Its first and second derivatives, indeed, provide respectively the *group velocity* and the *diffusion coefficient* of particle states.

### B. Coarse-graining of QWs

Our aim is to study scalar QWs on some group  $G$  containing  $H \cong \mathbb{Z}$  as a subgroup, with finitely many cosets in  $G$ . The minimal choice is  $G = H \cup Hr$ , where  $r$  is a coset representative. The group  $G$  is then virtually Abelian by definition. As a consequence, one can apply the coarse-graining procedure presented in Ref. [23] and study the kinematics of the walk in the  $k$ -space, likewise in the purely Abelian case.

This technique is applied through a unitary transformation on the walk operator: it is nothing but a change of representation of the generators of  $G$ , allowing one to represent the QW on  $G$  as a coarse-grained QW on  $H$  having larger coin system. In particular, two different choices of the subgroup  $H$  do not change the dispersion relations, which are informative about the kinematics of the system.

The core idea is to choose a partition of  $G$  into cosets of  $H$ , assigning to them a finite set of labels. The vertexes of the original Cayley graph of  $G$  are grouped into clusters—containing one vertex from each coset—which become the vertexes of the new coarse-grained walk on  $H$ . The coset labels designate now an additional internal degree of freedom.

A virtually Abelian quantum walk on  $\ell^2(G) \otimes \mathbb{C}^s$  can be regarded as an Abelian QW on  $\ell^2(H) \otimes \mathbb{C}^{s \times l}$ , where  $l$  is the index of  $H$  in  $G$ . In the present case,  $s = 1$  and  $l = 2$ . The coarse-graining procedure is performed by choosing a *regular tiling*, namely a particular coset partition of  $G$  with respect to an Abelian subgroup  $H$  of finite index. Accordingly, we will choose  $G = Hc_1 \cup Hc_2$ , with  $H \cong \mathbb{Z}$  and  $c_1, c_2$  arbitrary coset representatives.

We will denote the generators of  $G$  by  $h \in S_+$ . Having chosen the coset representatives  $\{c_j\}_{j=1,2}$ , we can define a unitary mapping between  $\ell^2(G)$  and  $\ell^2(H) \otimes \mathbb{C}^2$  as follows

$$U_H : \ell^2(G) \rightarrow \ell^2(H) \otimes \mathbb{C}^2; U_H |xc_j\rangle = |x\rangle |j\rangle, \forall x \in H,$$

for  $j = 1, 2$ . In Ref. [23] it is shown that—since  $\forall x \in H, \forall h \in S_+$  and  $\forall c_j$  there exist  $x' \in H$  and  $j' = \tau(h, j) \in \{1, 2\}$  such that  $xc_j h^{-1} = x' c_{j'}$ —the coarse-grained generating set  $\tilde{S}_+ = \{\tilde{h}\} \subseteq H$  is defined as

$$\tilde{S}_+ := \{c_{\tau(h,j)} h c_j^{-1} | h \in S, j = 1, 2\}, \quad (3)$$

while their corresponding transition matrices will be

given by

$$(A_{\tilde{h}})_{ij} = \sum_{h \in S_+} z_h \delta_{\tilde{h}, c_i h c_j^{-1}} \delta_{i, \tau(h, j)}. \quad (4)$$

Finally, the coarse-grained evolution operator reads

$$\begin{aligned} \mathcal{R}[A] &= (U_H \otimes \mathbb{K}) A (U_H \otimes \mathbb{K})^\dagger = \\ &= \sum_{h \in S_+} \sum_{j=1,2} T_{c_{\tau(h,j)} h c_j^{-1}} \otimes |\tau(h, j)\rangle \langle j| z_h, \end{aligned}$$

where clearly now  $T$  is the right regular representation of  $H$ . We say that a QW  $A$  is a *coarse-grained scalar QW* if there exists a scalar walk  $A'$  such that  $A = \mathcal{R}[A']$ .

It is known [3] that the only scalar QWs on  $\mathbb{Z}$  are the monoidal QW  $A_\pm := e^{-i\theta_\pm} T_\pm$ , with  $\theta_\pm$  arbitrary phases, and  $T_\pm$  the right/left shift operators on  $\ell^2(\mathbb{Z})$ . Here we analyze scalar QWs on a group that is virtually Abelian with Abelian subgroup  $H \cong \mathbb{Z}$ , starting from the easiest case in which the index of  $H$  is 2. Furthermore, we require the coarse-grained QW on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$  to have coordination number two, which restricts the class of Cayley graphs of  $G$  that we will study. Our analysis will lead to a classification of all the spinorial QW with coordination number 2 on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$  that can be obtained as a coarse-grained scalar QW.

The coarse-graining technique will be applied in Secs. IV A and IV B. In the following Section we classify infinite Abelian scalar QWs.

### III. CLASSIFICATION OF INFINITE ABELIAN SCALAR QWS ON CAYLEY GRAPHS

By the *fundamental theorem of finitely generated Abelian groups*, the generic infinite group of this kind is of the form  $G = \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d$ , for  $d \geq 1$  and  $0 \leq n < \infty$ . We now give a full characterization of infinite Abelian scalar QWs, providing a general structure for the evolution operator of these walks in the following Proposition.

**Proposition 1.** *Let  $A$  be the unitary operator of a scalar QW on the Cayley graph of  $G = \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d$  for  $1 \leq d < \infty$ , and  $0 \leq n < \infty$ . Then  $A$  splits into the direct sum of one-dimensional monoidal QWs  $e^{-i\theta_j} T_j$ , with  $T_j$  shift operators over  $\mathbb{Z}^d$ , and  $j \in \{1, 2, \dots, i_1 \times i_2 \times \dots \times i_n\}$ . In particular, the dispersion relations are linear in the wave-vectors.*

*Proof.* Let us pose  $G = \mathbb{Z}_{i_1} \times \dots \times \mathbb{Z}_{i_n} \times \mathbb{Z}^d =: F \times \mathbb{Z}^d$ , for  $d \geq 1$ . We can decompose the elements of  $G$  into one component in  $F$  and one in  $\mathbb{Z}^d$ ; accordingly, for some  $h \in S_+ \subset \mathbb{Z}^d$ , we define  $R(h) \subseteq F$  such that  $\bigcup_{h \in S_+} R(h) \times \{h\}$  is a set of generators for  $G$ . Let  $C_l$  be the right regular representation of the generator of  $\mathbb{Z}_{i_l}$  [32]. Then, defining for any  $f \in F$  the integers  $m_l(f) \in \{1, \dots, i_l\}$  such that  $T_f = C_1^{m_1(f)} \otimes \dots \otimes C_n^{m_n(f)}$ , the diagonalization

of the general QW on  $\ell^2(G) \otimes \mathbb{C}$  reads

$$\begin{aligned} A &= \sum_{h \in S_+} \sum_{f \in R(h)} (T_f \otimes T_h) z_{(f,h)} = \\ &= \sum_{j_1=1}^{i_1} \dots \sum_{j_n=1}^{i_n} |j_1\rangle \langle j_1| \otimes \dots \otimes |j_n\rangle \langle j_n| \otimes \sum_{h \in S_+} T_h z_h(\mathbf{j}), \end{aligned} \quad (5)$$

where

$$z_h(\mathbf{j}) := \sum_{f \in R(h)} z_{(f,h)} e^{2\pi i \left( j_1 \frac{m_1(f)}{i_1} + \dots + j_n \frac{m_n(f)}{i_n} \right)},$$

and  $\mathbf{j} := (j_1, \dots, j_n)$ . The evolution operator (5) is now block-diagonalizable in the  $k$ -space as

$$\int_{\mathcal{B}} d\mathbf{k} |\mathbf{k}\rangle \langle \mathbf{k}| \left( \sum_{\mathbf{h} \in S_+} e^{-i\mathbf{k} \cdot \mathbf{h}} z_{\mathbf{h}}(\mathbf{j}) \right), \forall \mathbf{j},$$

with  $A_{\mathbf{k}}(\mathbf{j}) := \sum_{\mathbf{h}} e^{-i\mathbf{k} \cdot \mathbf{h}} z_{\mathbf{h}}(\mathbf{j})$  unitary by construction. This leads to the unitarity conditions (2). Take now, for  $\mathbf{h}_i, \mathbf{h}_j \in S_+$ , the collection  $M$  of all the  $\mathbf{v} = \mathbf{h}_i - \mathbf{h}_j \in \mathbb{Z}^d$  such that

$$\|\mathbf{v}\| = \max_{\mathbf{h}_i, \mathbf{h}_j \in S_+} \|\mathbf{h}_i - \mathbf{h}_j\|. \quad (6)$$

Suppose that, for some  $\mathbf{v}' \in M$ , there exist two distinct pairs such that

$$\mathbf{v}' = \mathbf{h}_1 - \mathbf{h}_2 = \mathbf{h}_3 - \mathbf{h}_4, \quad (7)$$

with  $\mathbf{v}' \neq 0$  (otherwise  $d = 0$ ). Then let's define  $\mathbf{d}_{ij} := \mathbf{h}_i - \mathbf{h}_j$ : by definition one has  $2\mathbf{v}' = \mathbf{d}_{14} + \mathbf{d}_{32}$  and

$$\begin{aligned} 2\|\mathbf{v}'\| &= \|\mathbf{d}_{14} + \mathbf{d}_{32}\| \leq \|\mathbf{d}_{14}\| + \|\mathbf{d}_{32}\| \leq \\ &\leq \|\mathbf{v}'\| + \|\mathbf{v}'\| = 2\|\mathbf{v}'\|, \end{aligned}$$

where we used the triangle inequality and the definition (6) of  $\mathbf{v}'$ . This implies that  $\mathbf{d}_{14} \propto \mathbf{d}_{32}$  and  $\|\mathbf{v}'\| = \|\mathbf{d}_{14}\| = \|\mathbf{d}_{32}\|$ , which in turn imply  $\mathbf{d}_{14} = \pm \mathbf{d}_{32}$ ; this, combined with (7) and  $\mathbf{v}' \neq 0$  finally gives

$$\mathbf{h}_1 = \mathbf{h}_3, \quad \mathbf{h}_2 = \mathbf{h}_4,$$

i.e. the pair is unique. Then, by the unitarity conditions (2), one has  $z_{\mathbf{h}_1}(\mathbf{j}) z_{\mathbf{h}_2}^*(\mathbf{j}) = 0$ , namely e.g.  $z_{\mathbf{h}_1}(\mathbf{j}) = 0$ . The above argument can thus be iterated removing  $\mathbf{h}_1$  from the set  $S_+$ : one finally concludes that, for each  $\mathbf{j}$ , just one transition scalar  $z_{\tilde{\mathbf{h}}(\mathbf{j})}(\mathbf{j})$  is nonvanishing, namely

$$A_{\mathbf{k}}(\mathbf{j}) = \sum_{\mathbf{h} \in S_+} \delta_{\tilde{\mathbf{h}}(\mathbf{j}), \mathbf{h}} z_{\mathbf{h}}(\mathbf{j}) e^{-i\mathbf{k} \cdot \mathbf{h}} = z_{\tilde{\mathbf{h}}(\mathbf{j})}(\mathbf{j}) e^{-i\mathbf{k} \cdot \tilde{\mathbf{h}}(\mathbf{j})},$$

with  $z_{\tilde{\mathbf{h}}(\mathbf{j})}(\mathbf{j}) = e^{-i\theta_{\tilde{\mathbf{h}}(\mathbf{j})}}$  arbitrary phase factor (by unitarity of  $A_{\mathbf{k}}(\mathbf{j})$ ). We now conveniently define  $\mathbf{h}_j := \tilde{\mathbf{h}}(\mathbf{j})$ ,  $\theta_j := \theta_{\tilde{\mathbf{h}}(\mathbf{j})}$  and substitute in (5). Thus we finally

conclude that any infinite Abelian scalar QW is given by the direct sum of scalar walks on  $\mathbb{Z}$ , namely

$$A = \bigoplus_{j \in I} e^{-i\theta_j} T_j,$$

or else, in the Fourier representation

$$A = \int_{\mathcal{B}} d\mathbf{k} \bigoplus_{j \in I} e^{-i(\mathbf{k} \cdot \mathbf{h}_j + \theta_j)} \otimes |\mathbf{k}\rangle \langle \mathbf{k}|,$$

for  $I = \{1, 2, \dots, i_1 \times i_2 \times \dots \times i_n\}$  and with  $\mathbf{h}_j \in S_+ \subset \mathbb{Z}^d$ ,  $\theta_j$  arbitrary phases. This finally proves that the dispersion relations are linear in  $\mathbf{k}$ .  $\square$

Notice that the argument of the proof does not hold in the case of a general scalar QW on a finite Abelian group  $F$ . For example, it's easy to verify that the Cayley graph corresponding to  $\mathbb{Z}_2 \times \mathbb{Z}_2 = \langle g_1, g_2 | g_1^2, g_2^2, g_1 g_2 g_1^{-1} g_2^{-1} \rangle$  (square graph) admits a nontrivial scalar quantum walk.  $\square$

#### IV. SCALAR QWS ON THE INFINITE DIHEDRAL GROUP

##### A. Classification of the Cayley graphs

We provided a full classification of infinite Abelian scalar QWs. Accordingly, in the following we will consider just non-Abelian scalar QWs. We now aim to derive all the possible non-Abelian groups  $G \cong \mathbb{Z} \cup \mathbb{Z}r$  and their Cayley graphs satisfying the quadrangularity condition.

It is easy to show that an index-2 subgroup is always normal: by contradiction, let  $G$  be an arbitrary group and  $H$  be a index-2 subgroup which is not normal in  $G$ . Accordingly, for some  $x_1, x_2 \in H$ , the relation  $rx_1r^{-1} = x_2r$  holds, and this implies  $rx_1 = x_2r^2$ . However  $r^2$  must be equal to some  $xr$ , with  $x \in H$ , otherwise from the previous equation one would have  $r \in H$ . On the other hand,  $r^2 = xr$  reads  $r = x \in H$ , which is absurd. Then an index-2 subgroup is always normal: left and right cosets coincide. We conventionally choose right cosets to perform the coarse-graining.

Choosing  $G$  to be non-Abelian, let us pose  $H = \langle a \rangle$ : one has  $rar^{-1} = a^m$  for some integer  $m \neq 0, 1$  (by normality of  $H$ ); then  $a = r^{-1}a^m r = (r^{-1}ar)^m = a^{lm}$ , for  $l = \frac{1}{m}$  integer: the only possibility is  $m = -1$ . Thus we have  $rar^{-1} =: \varphi(a) = a^{-1}$ . Now we prove that  $r^2 = e$ . Indeed, it must be  $r^2 \in H$ . Let's now suppose that  $r^2 = a^p$ : then one has  $r^{-1}a^p = a^p r^{-1} = r^{-1}a^{-p}$ , implying  $p = 0$  and finally  $r^2 = e$ . Accordingly, since defining  $C = \langle r | r^2 \rangle$  one has  $G = HC$  and  $H \cap C = \{e\}$ , it follows that

$$G = H \rtimes_{\varphi} C \cong \mathbb{Z} \rtimes_{\varphi} \mathbb{Z}_2 = D_{\infty},$$

namely the infinite dihedral group, with the inverse map  $\varphi$  being the only nontrivial automorphism of  $\mathbb{Z}$  that achieves the semidirect product with  $\mathbb{Z}_2$ .



Since the cosets are mutually disjoint (they define equivalence classes), the elements of each coset of  $H$  in  $G$  define a distinct subset of vertexes of a Cayley graph of  $G$ ; in fact, the union of these subsets fills all the vertexes associated to the Cayley graph of  $G$ . Each element of  $H$  is in one-to-one correspondence with an element of  $Hr$  through elements of the form  $a^n r$ .

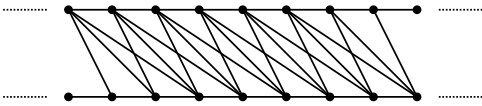
We now derive the admissible Cayley graphs of  $D_\infty$  satisfying the quadrangularity condition of Lemma 1. In order to find the coarse-grained generators  $\tilde{h}$ , one has to explicitly compute the set  $\tilde{S}_+$  in Eq. (3). The  $\tilde{h}$  depend in general on the cosets representatives (which are arbitrary): accordingly, we shall pose a general form  $c_1 = a^m, c_2 = a^{m'} r$ .

We are interested in walks represented on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$  with coordination number 2. Correspondingly, for the coarse-grained generators, we shall impose the condition

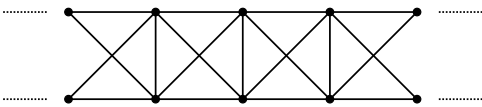
$$\tilde{h} \in \{e, a, a^{-1}\}. \quad (8)$$

We will then exclude the case  $a^l \in S_+$  with  $|l| \geq 2$ , since by (3), choosing for example  $j = 1$  one would have  $\tilde{h} = a^l$  which would give rise to coarse-grained walks with coordination number larger than two. Moreover, we can always include  $e$  in  $S_+$ , since by (3) the identity element is invariant under coarse-graining.

**Case  $a \in S_+$ .** All the generators beside  $a$  and  $e$  belong to the coset  $Hr$ , and are thus of the form  $a^n r$ . Moreover, combining (3) and (8), we must have  $|n - (m' - m)| \leq 1$ , namely  $h \in \{a^{(m' - m)} r, a^{(m' - m) + 1} r, a^{(m' - m) - 1} r\}$ . By quadrangularity, we need some generators  $h, h' \in Hr$  such that  $a^2 = hh'^{-1}$ , implying that  $a^{(m' - m) \pm 1} r \in S_+$ . Moreover, since  $h'h^{-1} = a^{-2}$  by quadrangularity it is also  $a^{-1} \in S_+$ . We can possibly include  $a^{(m' - m)} r$  in  $S_+$ , having  $e$  as coarse-grained generator. However, it is easy to check that  $\forall m, m'$  these choices give rise, topologically, to the same Cayley graph (modulo a constant left-translation  $a^{(m' - m)}$ ). Here it follows an example for the choice  $m' - m = 2$  (one moves between sites horizontally through  $a^{\pm 1}$ , while vertically through  $r$ , which has no associated edges in this example):



Accordingly, one can just set  $m = m' = 0$ , namely:



**Case  $a \notin S_+$ .** From the previous case we know that  $a \in S_+ \Leftrightarrow a^{-1} \in S_+$ , then obviously  $a \notin S_+ \Rightarrow a^{-1} \notin$

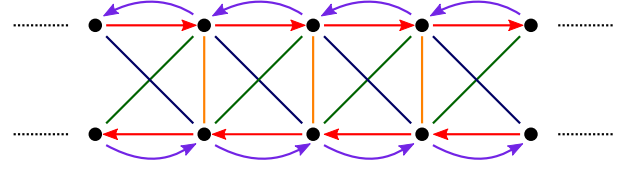


Figure 1. (colors online) The most general Cayley graph of the infinite dihedral group which admits a scalar QW with coarse-graining on  $\mathbb{Z}$  with coordination number two. The group presentation is:  $D_\infty = \langle a, a^{-1}, b, c, d | aa^{-1}, b^2, c^2, bda^{-1}, cda, bab^{-1}a, cac^{-1}a, bca^{-2} \rangle$ . The generators—namely  $a$  (red),  $a^{-1}$  (violet),  $b$  (dark blue),  $c$  (green) and  $d$  (orange)—are associated to edges of the graph, each corresponding to a transition scalar of the walk. Another Cayley graph of  $D_\infty$  with the same properties can be obtained by dropping  $d$  and the relators containing it. Moreover, one can include  $e$  in the generating set, which would correspond to a loop at each site.

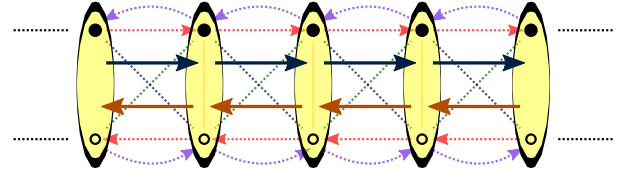


Figure 2. (colors online) Realization of the scalar QW in Fig. 1 as a quantum walk on  $\mathbb{Z} = \langle a, a^{-1} | aa^{-1} \rangle$  with a two-dimensional coin system. The original vertexes are grouped into pairs, realizing an additional helicity degree of freedom, and each edge—namely  $a$  (dark blue) and  $a^{-1}$  (brown)—is associated to a transition matrix. The cosets are associated to an element of a basis for  $\mathbb{C}^2$ : we choose the canonical basis, that is  $c_1 \rightarrow (1, 0)$  (full circles) and  $c_2 \rightarrow (0, 1)$  (empty circles).

$S_+$ . Then  $S_+ \subseteq \{e, h_i = a^{n+i} r | i = -1, 0, 1\}$ . However, for any pair  $(h_i, h_j)$  with  $i \neq j$ , there does not exist a different pair  $(h, h')$  such that  $hh'^{-1} = h_i h_j^{-1} = a^2$ , thus violating quadrangularity. This rules out the case  $a \notin S_+$ .

Colouring consistently the graph derived, one finds the most general admissible Cayley graph of  $D_\infty$ , which is shown in Fig. 1 together with the corresponding presentation.

## B. Classification of the scalar QWs

The scalar QWs on  $D_\infty$  are derived in Appendix A. The transition matrices of the coarse-grained QWs, computed choosing  $\{|1\rangle, |2\rangle\}$  to be the canonical basis of  $\mathbb{C}^2$  and using equations (4), are:

$$A_{+a} = \begin{pmatrix} z_a & z_b \\ z_c & z_{a^{-1}} \end{pmatrix}, \quad A_{-a} = \begin{pmatrix} z_{a^{-1}} & z_c \\ z_b & z_a \end{pmatrix}, \quad A_e = \begin{pmatrix} z_e & z_d \\ z_d & z_e \end{pmatrix}.$$

In Fig. 2 one finds a graphical scheme of the coarse-graining. Given  $A_k := e^{-ik}A_{+a} + e^{ik}A_{-a} + A_e$ , since the  $z_h$  are defined up to an overall phase factor, one can always take  $A_k \in \text{SU}(2)$ .

The solutions of the unitarity conditions (see Appendix A) give that the coarse-grained scalar QWs are of the form

$$A_k = e^{i\theta\sigma_x} A_k^D e^{i\theta'\sigma_x}, \quad (9)$$

with  $\theta, \theta' \in (-\pi/2, 0) \cup (0, \pi/2)$ , and  $A_k^D$  is the Dirac QW in one space dimension [14]

$$A_k^D = \begin{pmatrix} \nu e^{-ik} & i s \mu \\ i s \mu & \nu e^{ik} \end{pmatrix}, \quad \nu^2 + \mu^2 = 1, \quad s = \pm 1. \quad (10)$$

We denote by  $\mathcal{W}_{CG}$  the set of coarse-grained scalar QWs, i.e. the QWs  $A'_k$  such that  $A'_k = U A_k U^\dagger$  with  $A_k$  obeying Eq. (9) and  $U$  being a local change of basis—say  $U$  does not depend on  $k$ .

Let us now consider parity invariant QWs  $A_k^P$  on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ , i.e.

$$P A_k^P P^\dagger = A_{-k}, \quad P = P^\dagger = P^{-1},$$

where  $P$  gives a unitary representation in  $\mathbb{C}^2$  of the parity transformation. Assuming that the parity is not represented trivially, namely  $P \neq I$ , following the technique of Ref. [15] one obtains the full characterization of the class of parity invariant QWs:

$$A_k^P = U A'_k U^\dagger, \quad A'_k = e^{i\varphi\sigma_x} A_k^D, \quad (11)$$

with  $\varphi \in [-\pi/2, \pi/2]$ , and  $U$  a local change of basis. It is immediate to observe that the walk  $e^{i\varphi\sigma_x} A_k^D$  is parity invariant with  $P = \sigma_x$ .

We denote by  $\mathcal{W}_P$  the set of parity invariant QWs, and we observe that this set coincided with  $\mathcal{W}_{CG}$ . We have then proved the following result.

**Proposition 2.** *The set of coarse-grained scalar QWs with coordination number two on  $D_\infty$  coincides with the set of parity invariant QWs on  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ .*

We notice that the parity symmetry is inherited, in the coarse-graining procedure, from the particular automorphism  $\varphi$  realizing the semidirect product  $\mathbb{Z} \rtimes_\varphi \mathbb{Z}_2$ , which in this case is the inverse map. The popular Hadamard walk [4], which is not parity invariant, cannot be obtained by the coarse-grained of scalar QW.

The dispersion relations of the parity invariant QWs are of the form  $\pm\omega(k)$ , with

$$\omega(k) = \arccos(\delta \cos k + \gamma), \quad (12)$$

$$\delta, \gamma \in \mathbb{R}, |\delta \pm \gamma| \leq 1.$$

For any value of  $\gamma, \delta$ , the minimum of  $\{\omega(k), -\omega(k)\}$  is always attained at  $k_0 = 0$ , and that around  $k_0$  the behaviour can be either flat, or  $\pm|k|$  plus a constant, or smooth. We notice that when  $\gamma = 0$  we recover (up to a

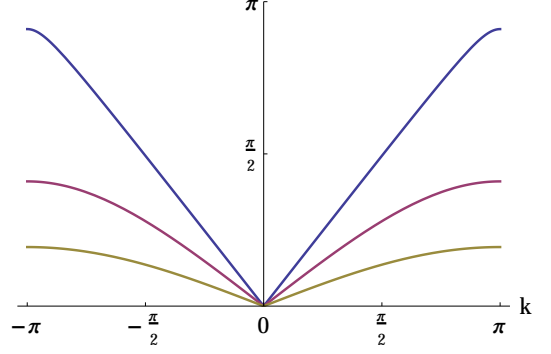


Figure 3. (colors online, the quantities plotted are dimensionless) Plot of  $\omega(k) = \arccos(\delta \cos k + \gamma)$ , for (from top to bottom)  $\delta = 0.98, 0.36, 0.09$  and  $\delta + \gamma = 1$ . This class of QWs exhibits, for  $|k| \approx 0$  and positive  $\delta$ , a massless (Weyl) dispersion relation (up to a rescaling of  $k$ ):  $\omega(k) \approx \delta|k|$ . For  $|k| \approx \pi$ ,  $\omega(k)$  becomes dispersive (massive).

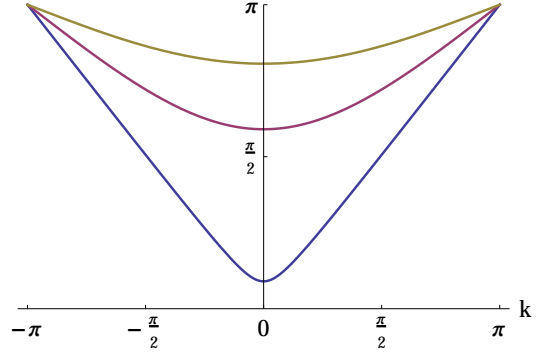


Figure 4. (colors online, the quantities plotted are dimensionless) Plot of  $\omega(k) = \arccos(\delta \cos k + \gamma)$ , for (from bottom to top)  $\delta = 0.98, 0.36, 0.09$  and  $\delta - \gamma = 1$ . This class of QWs exhibits a massive dispersion relation for  $|k| \approx 0$ , and a massless one for  $|k| \approx \pi$ . The Dirac dispersion relation is recovered for  $|k| \approx 0$  and  $\delta \approx 1$ . Notice that these dispersion relations are the same as those in Fig. 3, apart from a transformation  $\omega(k) \rightarrow \pi - \omega(k + \pi)$ .

local change of basis) the Dirac QW  $A_k^D$ . When  $\delta = 1$  we recover the Weyl QW  $A_k = \exp(-ik\sigma_z)$  which describes the dynamics of massless particles with a dispersion relation which is linear in  $k$ . We notice that when  $\delta + \gamma = 1$  the QW exhibits a non-dispersive behaviour for  $|k| \approx 0$  and a dispersive behaviour for greater values of  $|k|$ . The dispersion relations (12) are plotted for some values of the parameters  $\delta, \gamma$  in Figs. 3,4.

## V. CONCLUSIONS

We reviewed the notion of *quantum walk on Cayley graph* with the focus on scalar QWs. We also reviewed a coarse-graining technique that allows to unitarily map

a scalar QW on a virtually Abelian group to a coined QW on an Abelian group, what we call a coarse-grained scalar QW.

The first result we found is a classification of infinite Abelian scalar QWs (on Cayley graphs with arbitrary presentations), which turn out to be trivial from a dynamical point of view, meaning that they are given by a finite direct sum of shift operators times a phase factor. In particular, this implies that this class of QWs does not exhibit a massive dispersion relation. This result extends the previous results of Ref. [28], concerning  $\mathbb{Z}^d$ .

We then investigated scalar QWs on the infinite dihedral group  $D_\infty$ , which is the unique non-Abelian group  $G$  that contains a subgroup  $H \cong \mathbb{Z}$  with index two. We first derived all the Cayley graphs of  $D_\infty$  that allow for a scalar QW. Then we classified all the admissible QWs over the above Cayley graphs.

We notice that the unitarity conditions for a QW involve relations among four generators: if one solves them for the dihedral group, the derived transition amplitudes are a solution also for the QWs defined over the dihedral groups  $\mathbb{Z}_n \rtimes_{\varphi} \mathbb{Z}_2 \forall n \geq 4$ , corresponding to the same presentation with the additional condition  $a^n = e$ . In general, transforming some non-cyclic elements into cyclic ones on infinite groups presentations allows one to recover QWs on finite groups starting from QWs on infinite ones.

Finally we have shown that the class of QWs corresponding to the coarse-grained scalar QWs over  $D_\infty$  coincides, up to a local change of basis, to the class of QWs over  $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$  that are invariant under parity transformation. In this class we find QWs whose dispersion relations can exhibit a massive behaviour.

Interestingly, the coarse-graining technique allows one to build a bridge relating scalar and spinorial quantum walks, studying the symmetries of the latter as inherited from the underlying Cayley graph. Existence conditions in scalar QWs are more selective than the spinorial ones, and one can't recover all possible spinorial QWs starting from a scalar one. For example the Hadamard QW, which is not parity invariant, cannot be obtained a coarse-graining of a scalar QW. On the speculative side, this shows the crucial role played by the coarse-graining in the emergence of parity symmetry and helicity in one dimension.

## ACKNOWLEDGMENTS

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## Appendix A: Derivation of the dihedral QWs

Considering the polar representation  $z_h = |z_h|e^{i\theta_h}$  for the transition scalars, from the unitarity conditions (2)

one has (possibly with vanishing  $z_d$  or  $z_e$ )

$$z_{a\pm 1}z_{a\mp 1}^* + z_gz_f^* = 0, \quad (\text{A1})$$

$$z_{a\pm 1}z_g^* + z_gz_{a\pm 1}^* = 0, \quad (\text{A2})$$

$$z_dz_e^* + z_ez_d^* + z_{a\pm 1}z_b^* + z_bz_{a\pm 1}^* + z_{a\mp 1}z_c^* + z_cz_{a\mp 1}^* = 0, \quad (\text{A3})$$

$$z_gz_e^* + z_ez_g^* + z_dz_{a\pm 1}^* + z_{a\pm 1}z_d^* = 0, \quad (\text{A4})$$

$$z_{a\pm 1}z_e^* + z_ez_{a\mp 1}^* + z_dz_g^* + z_fz_d^* = 0, \quad (\text{A5})$$

with  $g, f \in \{b, c\}$  and  $g \neq f$ . From eqs. (A2), it follows *e.g.*  $e^{i\theta_b} = t_1 e^{i\theta_{a-1}}$  and  $e^{i\theta_c} = t_2 e^{i\theta_a}$  ( $t_{1,2}$  arbitrary signs), while from (A1) one has:

$$|z_a||z_{a-1}| = |z_b||z_c|,$$

$$s_1 := t_1 = -t_2,$$

$$e^{i\theta} := e^{i\theta_a} = s_2 e^{i\theta_{a-1}},$$

which are consistent with all of the (A2).

Therefore, we can satisfy the previous conditions and the normalization in (2) arbitrarily defining some real parameters such that the transition scalars are given by:

$$\begin{aligned} z_a &= \nu\sqrt{p}\sqrt{q}e^{i\theta}, & z_{a-1} &= s_2\nu\sqrt{1-p}\sqrt{1-q}e^{i\theta}, \\ z_b &= s_2s_1i\nu\sqrt{p}\sqrt{1-q}e^{i\theta}, & z_c &= -s_1i\nu\sqrt{1-p}\sqrt{q}e^{i\theta}, \\ z_e &= \mu\alpha e^{i\theta_e}, & z_d &= \mu\beta e^{i\theta_d}, \end{aligned}$$

where  $p, q \in (0, 1)$ ,  $\mu \in [0, 1]$ ,  $\alpha \in [0, 1]$  and  $\nu := \sqrt{1-\mu^2}$ ,  $\beta := \sqrt{1-\alpha^2}$ .

*a. Case  $z_d = z_e = 0$  ( $\mu = 0$ ).* The (A3) are already satisfied, while eqs. (A4),(A5) turn out to be trivial. Finally, we conclude that the transition scalars are:

$$\begin{aligned} z_a &= \sqrt{p}\sqrt{q}e^{i\theta}, \quad z_{a-1} = s_2\sqrt{1-p}\sqrt{1-q}e^{i\theta}, \\ z_b &= s_2s_1i\sqrt{p}\sqrt{1-q}e^{i\theta}, \quad z_c = -s_1i\sqrt{1-p}\sqrt{q}e^{i\theta}. \end{aligned}$$

*b. Case  $z_e = 0$  ( $\alpha = 0$ ).* The (A3) are already satisfied. From (A4) one has  $e^{i\theta_d} = s_3ie^{i\theta}$ , while from (A5)

$$\begin{aligned} e^{2i\theta_d} &= -s_2e^{2i\theta} \Rightarrow s_2 = +1, \\ |z_b| &= |z_c|. \end{aligned}$$

We conclude that the transition scalars are (up to a global phase factor)

$$\begin{aligned} z_a &= \nu p, \quad z_{a-1} = \nu(1-p), \\ z_b &= s_1i\nu\sqrt{p}\sqrt{1-p}, \quad z_c = -s_1i\nu\sqrt{p}\sqrt{1-p}, \\ z_d &= s_3i\mu, \end{aligned}$$

for  $p, \mu \in (0, 1)$ .

*c. Case  $z_d = 0$  ( $\beta = 0$ ).* The (A3) are already satisfied. From (A4) one has  $e^{i\theta_e} = s'_3e^{i\theta} := -s_1s_3e^{i\theta}$  (this definition is convenient in view of the next case  $z_e, z_d \neq 0$ ). From (A5) one gets

$$\begin{aligned} e^{2i\theta_e} &= -s_2e^{2i\theta} \Rightarrow s_2 = -1, \\ |z_a| &= |z_{a-1}|. \end{aligned}$$

We thus conclude that the transition scalars are (up to a global phase factor)

$$z_a = \nu\sqrt{p}\sqrt{1-p}, \quad z_{a-1} = -\nu\sqrt{p}\sqrt{1-p}, \\ z_b = -s_1 i\nu p, \quad z_c = -s_1 i\nu(1-p), \quad z_e = -s_1 s_3 \mu$$

for  $p, \mu \in (0, 1)$ .

d. **Case**  $z_e, z_d \neq 0$  ( $\mu, \alpha, \beta \neq 0$ ). (A3) reads

$$z_d z_e^* + z_e z_d^* = 0 \Rightarrow e^{i\theta_e} = s_4 i e^{i\theta_d}.$$

Substituting in eqs. (A4), one has

$$s_1 s_2 s_4 |z_b| |z_e| \cos(\theta_d - \theta) = -|z_d| |z_a| \cos(\theta_d - \theta), \\ s_1 s_2 s_4 |z_c| |z_e| \cos(\theta_d - \theta) = |z_d| |z_{a-1}| \cos(\theta_d - \theta),$$

which can be satisfied only if  $\cos(\theta_d - \theta) = 0$ , implying that  $e^{i\theta_d} = s_3 i e^{i\theta}$ . From (A5) we have

$$s_1 |z_e| (|z_a| + s_2 |z_{a-1}|) = s_4 |z_d| (s_2 |z_b| - |z_c|). \quad (\text{A6})$$

Notice that a change of the sign  $s_1 s_4$  affects last equation just by a relabeling  $|z_a| \leftrightarrow |z_{a-1}|$  (if  $s_2 = -1$ ) or  $|z_b| \leftrightarrow |z_c|$  (if  $s_2 = +1$ ), under which the unitarity conditions are invariant: thus we can set  $s_1 s_4 = +1$ . From (A6), one has to impose a positivity condition according to the choice of  $s_2$ , i.e.  $|z_b| - |z_c| > 0$  or  $|z_{a-1}| - |z_a| > 0$ , which imply some conditions on the  $p, q$ . Finally, one also finds the expression of  $\alpha$  in terms of  $p, q$  and  $s_2$ . We conclude that the transition scalars are (up to a phase factor):

$$z_a = \nu\sqrt{p}\sqrt{q}, \quad z_{a-1} = s_2 \nu\sqrt{1-p}\sqrt{1-q}, \\ z_b = s_2 s_1 i\nu\sqrt{p}\sqrt{1-q}, \quad z_c = -s_1 i\nu\sqrt{1-p}\sqrt{q}, \\ z_e = -s_1 s_3 \mu\alpha, \quad z_d = s_3 i\mu\beta,$$

where  $\alpha = \sqrt{p}\sqrt{1-q} - s_2\sqrt{1-p}\sqrt{q}$  and  $p, q, \mu \in (0, 1)$ , while  $p > q$  if  $s_2 = +1$ ,  $(1-q) > p$  if  $s_2 = -1$ .

In Eq. (9) of Sec. IV B we posed  $\cos \theta := \sqrt{p}$ ,  $\sin \theta := -s_1\sqrt{1-p}$ ,  $\cos \theta' := \sqrt{q}$ ,  $\sin \theta' := s_1 s_2\sqrt{1-q}$ , in Eq. (10)  $s := s_2 s_3$ , and in Eq. (12)  $\delta := z_a + z_{a-1}$  and  $\gamma := z_e$ .

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